

Computer aided perturbation theory by cumulants: dimerized and frustrated spin 1/2 chain

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This paper demonstrates that a computer aided perturbation theory can easily be realized by use of a cumulant approach. In contrast to a recent alternative formulation on the basis of Wegner's flow equation method the present approach can be applied to systems with arbitrary Hilbert space. In particular an equidistant spectrum of the unperturbed part of the Hamiltonian is not needed. The method is illustrated in detail for dimerized and frustrated spin 1/2 chains for which the ground state energy is calculated up to seventh order perturbation theory.

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INTRODUCTION

Perturbation theory has proved very powerful for the investigation of problems which are not exactly solvable. Thus, a number of different schemes have been developed which are either based on canonical transformations (a well-known example is the Schrieffer-Wolff transformation [1]) or on projection technique [2]. Because of the increasing computer capacity one would like to perform such systematic perturbation expansions up to high orders by use of algebraic programmes. Recently developed computer aided algorithms are based on the flow equation method [3, 4, 5] and Takahashi's formulation [6] of standard perturbation theory. The latter approach was used to derive an effective spin Hamiltonian for high-temperature superconductors [7], whereas the flow equation method has been applied to a number of low-dimensional systems, see e.g. Refs. 8. However, the applicability of the flow equation method is restricted to cases for which the unperturbed Hamiltonian has an equidistant eigenvalue spectrum. Only then the involved set of differential flow equations can be integrated.

Recently, a systematic perturbation expansion for many-particle systems in terms of cumulants has been proposed by two of us [9]. This method is an projection approach and is based on the construction of effective Hamiltonians for low-energy properties. Besides the automatically preserved size consistency of extensive variables, this cumulant method offers compact expressions for the different orders of the perturbation theory. The main problem for the evaluation of cumulant expressions is to properly count the number of contributing configurations or 'diagrams' to each order. However, since the counting of configurations can be taken over by the computer, the cumulant approach is an ideal starting point for an algebraic computer aided evaluation of physical quantities. The aim of the present paper is to demonstrate how these ideas can be put into practice.

For the sake of comparability, let us consider a dimer-

ized and frustrated $S = 1/2$ spin chain

$$\begin{aligned}\mathcal{H} &= \mathcal{H}_0 + \mathcal{H}_1 \\ \mathcal{H}_0 &= J \sum_{j=1}^N \mathbf{s}_j^e \cdot \mathbf{s}_j^o \\ \mathcal{H}_1 &= J\lambda \sum_{j=2}^N \left\{ \mathbf{s}_j^e \cdot \mathbf{s}_{j-1}^o + \alpha (\mathbf{s}_j^e \cdot \mathbf{s}_{j-1}^e + \mathbf{s}_j^o \cdot \mathbf{s}_{j-1}^o) \right\}\end{aligned}\tag{1}$$

in the limit of strong dimerization. This model was recently also investigated in Ref. 8 by use of the flow equation method. In Eq. (1), \mathbf{s}_j^e (\mathbf{s}_j^o) denotes the spin at even (odd) site of dimer j . The unperturbed part \mathcal{H}_0 of the Hamiltonian (1) describes N uncoupled dimers. Therefore, its ground state is the product of singlets on all dimers, and the excited states of \mathcal{H}_0 can be classified with respect to the number of local triplets. The perturbation \mathcal{H}_1 describes exchange interactions between neighboring dimers. In literature, spin chains of type (1) have been used for some spin-Peierls compounds like CuGeO_3 or TTFCuBDT [10, 11, 12]. Note that (1) is an example for a model with an equidistant unperturbed level scheme.

The paper is organized as follows. In the next section the cumulant approach [9] is formulated. In particular, the perturbation expansion of the resulting effective Hamiltonian is given in terms of cumulant expressions. In Sec. we develop the computer aided perturbation theory based on cumulants for the dimerized and frustrated $S = 1/2$ chain. The ground state energy is calculated up to seventh order in the interaction. This model is generalized in Sec. so that the spectrum of the unperturbed part \mathcal{H}_0 of the Hamiltonian becomes non-equidistant. Finally, the conclusions are presented in Sec. .

CUMULANT APPROACH

The cumulant approach [9] starts from the decomposition of the Hamiltonian $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$ into an unperturbed part \mathcal{H}_0 and into a perturbation \mathcal{H}_1 . The Hilbert

space of the unperturbed Hamiltonian \mathcal{H}_0 is split into two subspaces: The low-energy part \mathcal{U}_P and the high-energy part \mathcal{U}_Q with projection operators \mathcal{P} and $\mathcal{Q} = \mathbf{1} - \mathcal{P}$. Let us assume that the two subspaces are separated by a finite energy difference. It is our aim to construct an effective Hamiltonian for the low-energy subspace \mathcal{U}_P .

Motivated by the quantum statistical expression for the free energy, the effective Hamiltonian for the subspace \mathcal{U}_P is defined as follows

$$\mathcal{H}_{\text{eff}} = -\frac{1}{\beta} \mathcal{P} \ln (e^{-\beta \mathcal{H}})_P \mathcal{P} \quad (2)$$

where $(\cdots)_P$ denotes the operator product $\mathcal{P}(\cdots)\mathcal{P}$, β is the inverse temperature [9, 13]. Note that due to the projectors \mathcal{P} in Eq. (2) the effective Hamiltonian \mathcal{H}_{eff} only acts in the low-energy subspace \mathcal{U}_P .

In order to transform Eq. (2) into a cumulant expression we introduce generalized cumulants

$$\begin{aligned} (\mathcal{X}_1^{\nu_1} \cdots \mathcal{X}_N^{\nu_N})_P^C &\stackrel{\text{def}}{=} \\ &= \frac{\partial^{\nu_1}}{\partial \xi_1^{\nu_1}} \cdots \frac{\partial^{\nu_N}}{\partial \xi_N^{\nu_N}} \ln (e^{\xi_1 \mathcal{X}_1} \cdots e^{\xi_N \mathcal{X}_N})_P \Big|_{\xi_i=0 \ \forall i} \end{aligned} \quad (3)$$

which in contrast to usual cumulants [14, 15] are still operator quantities. A detailed discussion of generalized cumulants can be found in Ref. 9. By use of series expansions we transform the effective Hamiltonian (2) into a compact cumulant expression. Its Laplace transform can be used to derive a perturbation series for the effective Hamiltonian. For the case that all states of the relevant \mathcal{U}_P subspace are degenerate with respect to \mathcal{H}_0 , the resulting effective Hamiltonian reads at temperature $T = 0$

$$\begin{aligned} (\mathcal{T}_1 \cdots \mathcal{T}_M)_P^C &= (\mathcal{T}_1 \cdots \mathcal{T}_M)_P - \frac{1}{2} \sum_{\substack{n_1, \dots, n_M=0 \\ (n_1, \dots, n_M) \neq (0, \dots, 0)}}^1 \sum_{\substack{m_1, \dots, m_M=0 \\ (m_1, \dots, m_M) \neq (0, \dots, 0)}}^1 \delta(1, n_1 + m_1) \cdots \delta(1, n_M + m_M) \times \\ &\quad \times (\mathcal{T}_1^{n_1} \cdots \mathcal{T}_M^{n_M})_P (\mathcal{T}_1^{m_1} \cdots \mathcal{T}_M^{m_M})_P + \cdots \end{aligned} \quad (7)$$

Thus, the calculation of cumulant expressions is reduced to the evaluation of sums over operator products which can be easily done by use of a computer. The main limitation for a concrete realization is given by the increasing number of convoluted sums. Consequently, the numerical effort may be considerable, if additional restrictions have to be taken into account.

[9]

$$\begin{aligned} \mathcal{H}_{\text{eff}}(\beta \rightarrow \infty) &= \\ &= (\mathcal{H}_0)_P^C + \lim_{z \rightarrow 0} \left\{ \sum_{n=0}^{\infty} \left(\mathcal{H}_1 \left[\frac{1}{z - \mathbf{L}_0} \mathcal{H}_1 \right]^n \right)_P^C \right\}. \end{aligned} \quad (4)$$

Here, \mathbf{L}_0 is the Liouville operator with respect to \mathcal{H}_0 . It is defined by $\mathbf{L}_0 \mathcal{A} = [\mathcal{H}_0, \mathcal{A}]$ for any operators \mathcal{A} .

To calculate the cumulants in Eq. (4) one first decomposes the perturbation \mathcal{H}_1 into eigenoperators of \mathbf{L}_0

$$\mathcal{H}_1 = \sum_m \mathcal{T}_m \quad \text{with} \quad \mathbf{L}_0 \mathcal{T}_m = \Delta_m \mathcal{T}_m. \quad (5)$$

Due (5) also products of \mathcal{T}_m are eigenoperators of \mathbf{L}_0 [13]. Therefore, the energy denominators of Eq. (4) can directly be evaluated

$$\begin{aligned} \left(\mathcal{A} \frac{1}{z - \mathbf{L}_0} \mathcal{T}_1 \cdots \mathcal{T}_M \right)_P^C &= \\ &= \frac{1}{z - (\Delta_1 + \cdots + \Delta_M)} (\mathcal{A} \mathcal{T}_1 \cdots \mathcal{T}_M)_P^C. \end{aligned} \quad (6)$$

We are left with the calculation of cumulant expressions of the general form $(\mathcal{T}_1 \cdots \mathcal{T}_M)_P^C$. For this purpose, we rewrite the cumulant expression (3) by expanding the logarithm into powers of ξ_i and perform the differentiations. We find the following decomposition of the generalized cumulants into operator products [9]

DIMERIZED AND FRUSTRATED SPIN 1/2 CHAIN

In this section we show how the cumulant approach can be used to perform specific calculations. For this purpose we want to construct an effective Hamiltonian for the dimerized and frustrated spin 1/2 chain (1) in the limit of strong dimerization. As mentioned above, in this limit the unperturbed part \mathcal{H}_0 of the Hamiltonian describes isolated dimers without interaction between different dimers. Therefore, the low-energy subspace \mathcal{U}_P is given by a single state which is a product state formed

$4\mathcal{T}_0(j)$	
$ t^{0,\pm}, s\rangle \rightarrow$	$-J\lambda(1-2\alpha) s, t^{0,\pm}\rangle$
$ t^0, t^\pm\rangle \rightarrow$	$J\lambda(1+2\alpha) t^\pm, t^0\rangle$
$ t^\pm, t^\pm\rangle \rightarrow$	$J\lambda(1+2\alpha) t^\pm, t^\pm\rangle$
$ t^\pm, t^\mp\rangle \rightarrow$	$J\lambda(1+2\alpha)\{ t^0, t^0\rangle - t^\pm, t^\mp\rangle\}$
$ t^0, t^0\rangle \rightarrow$	$J\lambda(1+2\alpha)\{ t^+, t^-\rangle + t^-, t^+\rangle\}$
$4\mathcal{T}_1(j)$	
$ s, t^+\rangle, t^+, s\rangle \rightarrow$	$J\lambda\{ t^0, t^+\rangle - t^+, t^0\rangle\}$
$ s, t^0\rangle, t^0, s\rangle \rightarrow$	$J\lambda\{ t^-, t^+\rangle - t^+, t^-\rangle\}$
$ s, t^-\rangle, t^-, s\rangle \rightarrow$	$J\lambda\{ t^-, t^0\rangle - t^0, t^-\rangle\}$
$4\mathcal{T}_2(j)$	
$ s, s\rangle \rightarrow$	$J\lambda(1-2\alpha)\{ t^+, t^-\rangle + t^-, t^+\rangle + t^0, t^0\rangle\}$

TABLE I: Action of the $\mathcal{T}_m(j)$ as used in the calculations. For convenience, the dimer indices of the states are suppressed.

by singlets on all dimers. The low- and the high-energy subspaces are separated by the singlet-triplet splitting

$$\Delta = \varepsilon_t - \varepsilon_s = J \quad (8)$$

on a single dimer. Thus, the low-energy subspace \mathcal{U}_P only consists of a single state, i.e. the singlet product state. The effective Hamiltonian acting in \mathcal{U}_P can be directly identified with the ground-state energy of the complete

problem, multiplied by the projector \mathcal{P} .

Next we decompose the perturbation \mathcal{H}_1 into eigenoperators of the Liouville operator \mathbf{L}_0 . As mentioned above, the excited states of the unperturbed Hamiltonian \mathcal{H}_0 [see Eq. (1)] can be classified according to the number of local triplets. The creation and the annihilation of a local triplet state can be interpreted as the fundamental excitation processes. Therefore, also the eigenoperators of the Liouville operator can be classified by the number of local triplets and \mathcal{H}_1 can be rewritten as

$$\mathcal{H}_1 = \mathcal{T}_{-2} + \mathcal{T}_{-1} + \mathcal{T}_0 + \mathcal{T}_1 + \mathcal{T}_2. \quad (9)$$

An eigenoperator \mathcal{T}_m creates m local triplets. The respective eigenvalues of the Liouville operator are

$$\begin{aligned} \Delta_{-2} &= -2\Delta, & \Delta_{-1} &= -\Delta, & \Delta_0 &= 0, \\ \Delta_1 &= \Delta, & \Delta_2 &= 2\Delta. \end{aligned} \quad (10)$$

The perturbation \mathcal{H}_1 [see Eq. (1)] consists of interactions between adjacent dimers. Therefore, no further excitation operators occur, and the \mathcal{T}_m 's can be directly constructed from two-dimer matrix elements

$$\langle x_{j-1}, x_j | J\lambda \{ \mathbf{s}_j^e \cdot \mathbf{s}_{j-1}^o + \alpha (\mathbf{s}_j^e \cdot \mathbf{s}_{j-1}^e + \mathbf{s}_j^o \cdot \mathbf{s}_{j-1}^o) \} | y_{j-1}, y_j \rangle \quad (11)$$

where $x_{j-1}, y_{j-1}, x_j, y_j$ denote singlets (s) and triplets (t^-, t^0, t^+) on the dimers $(j-1)$ and j . Let us introduce local transition operators $\mathcal{T}_m(j)$ by the relation

$$\begin{aligned} \mathcal{T}_{-2}(j) + \mathcal{T}_{-1}(j) + \mathcal{T}_0(j) + \mathcal{T}_1(j) + \mathcal{T}_2(j) &= \\ &= J\lambda \{ \mathbf{s}_j^e \cdot \mathbf{s}_{j-1}^o + \alpha (\mathbf{s}_j^e \cdot \mathbf{s}_{j-1}^e + \mathbf{s}_j^o \cdot \mathbf{s}_{j-1}^o) \} \end{aligned} \quad (12)$$

which are again classified with respect to the net change of the number of triplets. Eqs. (12) together with (11) allows to construct the transition operators. For instance, matrix elements of (11) connecting two singlet states [on the dimers $(j-1)$ and j] with two triplet states [on the dimers $(j-1)$ and j] contribute to $\mathcal{T}_2(j)$. The results for $\mathcal{T}_0(j), \mathcal{T}_1(j), \mathcal{T}_2(j)$ are summarized in Tab. I. The remaining transition operators $\mathcal{T}_{-1}(j)$ and $\mathcal{T}_{-2}(j)$ follow from the relation $\mathcal{T}_{-m}(j) = \mathcal{T}_m^\dagger(j)$. The compact eigenoperators \mathcal{T}_m of the Liouville operator are given by

$$\mathcal{T}_m = \sum_{j=2}^N \mathcal{T}_m(j). \quad (13)$$

Note that the above decomposition of \mathcal{H}_1 was also derived in Ref. 8.

Now we can calculate the cumulant expressions

$$\begin{aligned} (\mathcal{T}_{m_1} \dots \mathcal{T}_{m_k})_P^C &= \\ &= \sum_{j_1=2}^N \dots \sum_{j_k=2}^N (\mathcal{T}_{m_1}(j_1) \dots \mathcal{T}_{m_k}(j_k))_P^C \end{aligned} \quad (14)$$

which enter the effective Hamiltonian (4). For that purpose it is favorable to exploit some additional restrictive conditions. In this way the number of contributions to the cumulants, which have to be calculated explicitly, can be considerably reduced. Remember, the effective Hamiltonian (4) acts in the low-energy subspace \mathcal{U}_P which is formed by the product state of singlets on all dimers. It follows

- (i) Products of the \mathcal{T}_m operators inside the cumulant expression do not change the number of triplets, i.e. $m_1 + m_2 + \dots + m_k = 0$ has to be fulfilled.
- (ii) Due to the explicit form of the excitation operators (see Tab. I), the low-energy subspace \mathcal{U}_P and the high-energy subspace \mathcal{U}_Q are only connected by \mathcal{T}_2 and \mathcal{T}_{-2} . Thus, non-vanishing contributions to (14) can only occur if $m_1 = -2$ and $m_k = 2$.

- (iii) Due to general properties of cumulants [14] only connected processes or 'diagrams' contribute to cumulant expressions. Therefore, the maximum range of connected dimers in (14) is restricted to

$$\begin{aligned} j_{\max} - j_{\min} &= \\ &= \max(j_1, \dots, j_k) - \min(j_1, \dots, j_k) \leq (k-1) \end{aligned} \quad (15)$$

All dimers between j_{\min} and j_{\max} enter the cumulant.

Whereas (i) and (ii) directly follow from Eqs. (14) and (7) the condition (iii) represents a basic feature of cumulant expressions. Note that these restrictive conditions extremely simplify the evaluation of the effective Hamiltonian (4). The zeroth order of \mathcal{H}_{eff} is given by $\mathcal{H}_0 = N\varepsilon_s \mathcal{P}$ whereas the first order contribution vanishes due to $(\mathcal{H}_1)_P = 0$. The second order contribution to the effective Hamiltonian reads

$$\begin{aligned} \mathcal{H}_{\text{eff}}(\beta \rightarrow \infty)|_{\text{2nd order}} &= - \left(\mathcal{H}_1 \frac{1}{\mathbf{L}_0} \mathcal{H}_1 \right)_P^C \\ &= - \frac{1}{2\Delta} (\mathcal{T}_{-2} \mathcal{T}_2)_P^C \end{aligned} \quad (16)$$

where we have used (ii). Now we insert Eq. (13) into (16) and take the condition (iii) into account. Thus

$$\begin{aligned} \mathcal{H}_{\text{eff}}(\beta \rightarrow \infty)|_{\text{2nd order}} &= \\ &= - \frac{1}{2\Delta} \sum_{j_1=2}^N \sum_{j_2=2}^N (\mathcal{T}_{-2}(j_1) \mathcal{T}_2(j_2))_P^C \\ &= - \frac{N}{2\Delta} (\mathcal{T}_{-2}(j) \mathcal{T}_2(j))_P^C \end{aligned} \quad (17)$$

where the dimer site index j can be chosen arbitrarily. Note that in (17) $(N-1)$ was approximated by N . The remaining cumulant in (17) can be easily evaluated by use of Eq. (7) and the matrix elements of Tab. I. We find

$$\mathcal{H}_{\text{eff}}(\beta \rightarrow \infty)|_{\text{2nd order}} = - \frac{3}{32} N \Delta \lambda^2 (1-2\alpha)^2 \mathcal{P}. \quad (18)$$

Next, we use the computer to calculate the higher orders of perturbation theory. By use of the computer algebra system Maple V [16] we have implemented the following steps:

- (a) At first, the decomposition (9) of the perturbation \mathcal{H}_1 is inserted in the cumulant expressions so that all energy denominators can be easily evaluated [compare with Eq. (6)]. Consequently, the cumulants of Eq. (4) are decomposed into sums of expressions of the form (14).
- (b) Cumulants of the form (14) are computed by use of Eq. (7) if the above conditions (i) - (iii) are fulfilled. Otherwise no further evaluation is needed.

- (c) Finally, the remaining operator products of Eq. (7) are calculated.

It is obvious that steps (a) and (b) can easily be implemented by use of computer loops. For the calculation of the operator products of Eq. (7) in step (c), it is sufficient to consider finite clusters. The finite order contribution of a short-ranged perturbation is independent from the cluster size if the cluster is chosen large enough. One can also prove explicitly that the results are not affected by the cluster size. A state of the cluster is described by an array of integers $\{1, 2, 3, 4\}$ which represent the states $\{s, t^+, t^0, t^-\}$ for each dimer. The \mathcal{T} operators applied to a cluster change the elements of the integer array which then describes the final cluster state. Finally, one has to count over all contributing processes.

As result of the computer aided perturbation theory we find the following effective Hamiltonian

$$\mathcal{H}_{\text{eff}}(\beta \rightarrow \infty) = -NJ \sum_n \left(\frac{\lambda}{4} \right)^n h_n \mathcal{P} \quad (19)$$

The parameters h_n up to seventh order read

$$\begin{aligned} h_0 &= \frac{3}{4}, \\ h_1 &= 0, \\ h_2 &= \frac{3}{2} (1-2\alpha)^2, \\ h_3 &= \left(\frac{3}{2} + 3\alpha \right) (1-2\alpha)^2, \\ h_4 &= \left(\frac{13}{8} + \frac{27}{2}\alpha - \frac{3}{2}\alpha^2 \right) (1-2\alpha)^2, \\ h_5 &= \left(\frac{89}{24} + \frac{311}{12}\alpha + \frac{93}{2}\alpha^2 - 45\alpha^3 \right) (1-2\alpha)^2, \\ h_6 &= \left(\frac{463}{48} + \frac{454}{9}\alpha + \frac{1307}{6}\alpha^2 - 84\alpha^3 - 159\alpha^4 \right) \times \\ &\quad \times (1-2\alpha)^2, \\ h_7 &= \left(\frac{81557}{3456} + \frac{257909}{1728}\alpha + \frac{215995}{432}\alpha^2 + \frac{173579}{216}\alpha^3 \right. \\ &\quad \left. - \frac{14865}{8}\alpha^4 + \frac{879}{4}\alpha^5 \right) (1-2\alpha)^2. \end{aligned} \quad (20)$$

Apart from the projector \mathcal{P} the effective Hamiltonian [(19) and (20)] can be directly identified as the ground-state energy of the original Hamiltonian (1). As discussed above, this follows from the fact that the low-energy subspace \mathcal{U}_P only consists of a single state. Note that the present result for the ground-state energy agrees with the result obtained before on the basis of the flow equation method [8].

THE GENERALIZED MODEL

The unperturbed part \mathcal{H}_0 of the Hamiltonian (1), which we have studied up to now, has had an equidistant spectrum. Note that this property of \mathcal{H}_0 was explicitly needed in the flow-equation approach to construct perturbative effective Hamiltonians [8]. In the following we want to demonstrate that this property of the model Hamiltonian is not required in the cumulant method discussed above. For that purpose let us modify the unperturbed Hamiltonian \mathcal{H}_0 of the model (1), whereas \mathcal{H}_1 is kept unchanged: The coupling between the two spins of each dimer is chosen to be different for dimers with even and odd site index j

$$\mathcal{H}_0 = J \sum_{j=1}^N \mathbf{s}_j^e \cdot \mathbf{s}_j^o + J\delta \sum_{j=1}^{N/2} \mathbf{s}_{2j}^e \cdot \mathbf{s}_{2j}^o. \quad (21)$$

Note that the new Hamiltonian \mathcal{H}_0 does not change the eigenstates of the previous unperturbed Hamiltonian (1). However, the eigenenergies are different. The dimer singlet and triplet energies depend on the dimer index j and are given by

$$\varepsilon_s(j) = \begin{cases} \varepsilon_s & j \text{ odd} \\ (1+\delta)\varepsilon_s & j \text{ even} \end{cases} \quad (22)$$

$$\varepsilon_t(j) = \begin{cases} \varepsilon_t & j \text{ odd} \\ (1+\delta)\varepsilon_t & j \text{ even} \end{cases} \quad (23)$$

Therefore, the spectrum of the unperturbed Hamiltonian \mathcal{H}_0 is not equidistant anymore. Due to the modification (21) of \mathcal{H}_0 also the Liouville operator \mathbf{L}_0 has changed. The decomposition of the perturbation \mathcal{H}_1 , Eq. (1), into transition operators with respect to \mathcal{H}_0 has to be modified too. In particular, the number of created local triplets can not be the only classification criterion anymore since the singlet-triplet splittings differs for different dimer sites. In fact, the former transition operators \mathcal{T}_1 , \mathcal{T}_0 , and \mathcal{T}_{-1} have to be split up. The perturbation \mathcal{H}_1 can now be written as

$$\mathcal{H}_1 = \mathcal{T}_{-2} + \mathcal{T}_{-1,-} + \mathcal{T}_{-1,0} + \mathcal{T}_{0,-} + \mathcal{T}_{0,0} + \mathcal{T}_{0,+} + \mathcal{T}_{1,0} + \mathcal{T}_{1,+} + \mathcal{T}_2 \quad (24)$$

and the respective eigenvalues of the modified Liouville operator now read

$$\begin{aligned} \Delta_2 &= (2+\delta)\Delta \\ \Delta_{1,+} &= (1+\delta)\Delta \\ \Delta_{1,0} &= \Delta \\ \Delta_{0,+} &= \delta\Delta \\ \Delta_{0,0} &= 0 \\ \Delta_{0,-} &= -\delta\Delta \\ \Delta_{-1,0} &= -\Delta \\ \Delta_{-1,-} &= -(1+\delta)\Delta \\ \Delta_{-2} &= -(2+\delta)\Delta \end{aligned} \quad (25)$$

The second index x in $\mathcal{T}_{\pm 1,x}$ and $\mathcal{T}_{0,x}$ denotes how the number of triplets on dimers with even index j is changed. ($x = +(-)$ describes the creation (annihilation) of a triplet and $x = 0$ no change). Note that the original model (1) is given by $\delta = 0$.

The next steps can be done as before. At first we introduce local transition operators. Furthermore, the restrictive conditions (a), (b), (c) are still valid so that the evaluation of the cumulants can be done similar as before. (Of course, now one has to distinguish between odd and even dimer indices.) By use of the computer aided perturbation theory we now find an effective Hamiltonian which has the form of expression (19). The parameters h_n , up to fourth order, now read

$$h_0 = \frac{3}{8}(2+\delta), \quad (26)$$

$$h_1 = 0,$$

$$h_2 = \frac{3}{(2+\delta)}(1-2\alpha)^2,$$

$$h_3 = \frac{4}{(2+\delta)^2} \left(\frac{3}{2} + 3\alpha \right) (1-2\alpha)^2,$$

$$h_4 = 3 \frac{(1-2\alpha)^2}{(2+\delta)^2} \left(12 \frac{2+\delta}{(3+2\delta)(3+\delta)} + \frac{(2+\delta)(1-2\delta)^2}{1+\delta} - \frac{5-52\alpha+20\alpha^2}{2+\delta} \right).$$

In fact, we have calculated the h_n also up to seventh order. Since the expressions are rather involved, here the h_n 's are only given up to the fourth order. Higher orders are available on request. Note that in the case of $\delta = 0$ Eq. (26) reduces to (20).

CONCLUSIONS

In this paper we have shown that a recently developed cumulant method [9] can be used to develop computer aided perturbation theory. Size consistency of extensive variables is fulfilled. The cumulant method offers compact expressions for the different orders of the perturbation theory. Furthermore, the evaluation of the cumulant expressions is reduced to the problem how to properly count the contributing processes.

We have applied the cumulant method to the dimerized and frustrated spin 1/2 chain. For this model the ground-state energy was calculated up to seventh order perturbation theory where our results agree with those obtained by the flow equation method [8]. It turned out that the efficiency of the computer based evaluation of the cumulant expressions can be enormously improved if restrictive conditions are considered. In this way the number of vanishing contributions in the calculations can be reduced. Furthermore, we have modified the model by

an additional site-oscillating dimer coupling so that the spectrum of the unperturbed part of the Hamiltonian is not equidistant anymore. For the generalized model we have calculated the ground-state energy up to seventh order perturbation theory as well. Note that in contrast to the cumulant approach the flow equation method used in Ref. 8 requires an equidistant spectrum of the unperturbed part of the Hamiltonian. On the other hand, the flow equation method can also be used to calculate excitation energies.

The derivation of the cumulant expression (4) for the effective Hamiltonian $\mathcal{H}_{\text{eff}}(\beta \rightarrow \infty)$ was based on the assumption that it is acting in the lowest energy subspace \mathcal{U}_P of \mathcal{H}_0 . This subspace can either be degenerate or nondegenerate. For the dimerized spin 1/2 chain the lowest energy subspace is one-dimensional and is given by the product of all dimer singlet states. An example for a degenerate unperturbed groundstate was discussed in Ref. 9. Note that the cumulant expression (4) is also closely related to an effective Hamiltonian which was derived by Takahashi [6]. There, the eigenvalue problem of the full Hamiltonian is transformed to that of an effective Hamiltonian which acts in a degenerate or nondegenerate energy subspace of \mathcal{H}_0 . By comparing the perturbation expansion (4) order by order with that of Ref. [6] the equivalence of both approaches can be shown. Takahashi's approach does not involve the temperature. Therefore, the subspace in which the effective Hamiltonian acts is not necessarily the lowest energy subspace of \mathcal{H}_0 . Thus, one might expect the cumulant result (4) should also be valid for this case which would allow to calculate excitation energies. Finally, a projector-based renormalization method (PRM) for effective Hamiltonians was recently introduced by two of the present authors [17]. By using perturbation theory also in this approach [18] a close relation to the cumulant expression (4) can be found. However, the PRM treatment seems to be more suited to calculate excitation energies than the cumulant approach presented here.

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